Structure of the GMI Code

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Abstract

In this report, we provide a brief description of the GMI code and give the directory structure of the code. In addition, we present a general flowchart of the code and routine sequence of the chemistry operator.

1- Overview of the Model

The Global Modeling Initiative (GMI) was initiated under the auspices of the Atmospheric Effects of Aircraft Program (AEAP) in 1995. The goal of GMI is to develop and maintain a state-of-the-art modular 3-D chemistry transport model (CTM) that can be used for assessment of the impact of various natural and anthropogenic perturbations on atmospheric composition and chemistry, including, but not exclusively, the effect of aircraft.

More recently, ACMAP has selected the approach of GMI to serve as both and assessment facility and a testbed for model improvements for future assessment in all areas of atmospheric chemistry.

The GMI model is a modular chemistry-transport model (CTM) with the ability to carry out multi-year assessment simulations as well as incorporate different modules, such as meteorological fields, chemical mechanisms, numerical methods, and other modules representing the different approaches of current models. This capability facilitates the understanding of the differences and uncertainties of model results.

The testing of GMI results against observations is a high priority of GMI activities. Science Team members contribute by either supplying a particular module and/or contributing to the analysis of the results and comparison with atmospheric observations [3, 5]. Application of the model to the potential impacts of stratospheric aircraft emissions is presented in [4]. The model was employed to investigate the effects of stratospheric aircraft emissions on the polar stratospheric clouds [1] and simulate ozone recovery over a 36-year time period [2].

Besides acting as a testbed for different modules, GMI will also act as a 3-D assessment facility. The GMI modular code is currently implemented at NASA/Goddard Space Flight Center (the core institution). The core institution is responsible for: integrating and testing component of the GMI model, maintaining coding standards which will make the model transportable to different platforms, carrying out assessment calculations, and

providing first-order results and diagnostics for analysis by team members. The current code has been developed to run on a variety of computing platforms, both with single and multiple processors (SGI Origin series, HP Compaq SC45, Beowulf clusters, etc.).

2- Components of GMI

The modules that make up the GMI assessment model are [5]:

1. Input meteorological data coming from three major Global Circulation Models (from NCAR, GISS and DAO). Data from all these input sets included horizontal U and V winds, temperature, and surface pressure.
2. Advection algorithm to transport trace species
3. Mass tendencies
4. Numerical schemes for chemistry solutions
5. Chemistry mechanism
6. Heterogeneous processes
7. Photolysis
8. Diagnostics
9. Tropospheric treatment
10. Initial conditions
11. Boundary conditions

All the above modules have multiple options.

3- Directory Structure of The Code

The top directory of the GMI code is *gem/* which contains the sub-directories

- *actm/*: for the atmospheric transport model
- *bin/*: location of the code executable
- *doc*/: general information about the code and how it is to be used
- *esm*/: Earth System Modeling package
- *esm_tools*/: tools for the ESM package
- *include*/: general-purpose head files for platform selection, compilation selection, message passing options, etc.

In Tables 1, 2, 3, and 4, we give more details on the structure of each of the above sub-directories.

Sub-directories	Description
actm	Atmospheric Chemistry Transport Model
actm/gmimod	
actm/gmimod/Other	
actm/gmimod/Other/doc	README files
actm/gmimod/Other/misc	
actm/gmimod/Other/scripts	Script files performing various functions

actm/gmimod/Other/test	Basic test cases to run the model
actm/gmimod/Other/test/nopar	
actm/gmimod/Other/test/nopar/Old	
actm/gmimod/Other/test/nopar/infiles	Sample input namelist files
actm/gmimod/Other/test/nopar/outfiles	ASCII output files for the test cases in infiles/
actm/gmimod/Other/test/par	
actm/gmimod/Other/test/par/infiles	Sample input namelist files
actm/gmimod/Other/test/par/outfiles	ASCII output files for the test cases in infiles/

Table 1: *GMI code directories I*

Subdirectories	Description
actm/gmimod/advec	Advection operator module
actm/gmimod/advec/dao2advec	DAO advection routines
actm/gmimod/advec/dao2utils	Advection utility routine computing courant numbers, Divergence, etc.
actm/gmimod/advec/include	Advection include file
actm/gmimod/chem	Chemistry operator package
actm/gmimod/chem./aerosol	Aerosol chemistry
actm/gmimod/chem./aerosol/include_setkin	Include files for aerosol
actm/gmimod/chem./aerosol/setkin	Routines for rate constants and rates of kinetic processes calculations
actm/gmimod/chem./include	Chemistry include file
actm/gmimod/chem./sad	Aerosol surface area density and condensed phase mixing ratio modules
actm/gmimod/chem./smv2chem	Chemistry solver routines
actm/gmimod/chem./stratosphere	Stratospheric chemistry
actm/gmimod/chem./stratosphere/include_setkin	Include files for stratosphere
actm/gmimod/chem./stratosphere/setkin	Routines for rate constants and rates of kinetic processes calculations
actm/gmimod/chem./sulfur	Routines for sulfur chemistry
actm/gmimod/chem./troposphere	Tropospheric chemistry
actm/gmimod/chem./troposphere/include_setkin	Include files for troposphere
actm/gmimod/chem./troposphere/setkin	Routines for rate constants and rates of kinetic processes calculations

Table 2: *GMI code directories II*

Sub-directories	Description
actm/gmimod/comm	MPI communication routines
actm/gmimod/control	Routines defining ACTM procedures (init, advance, final)
actm/gmimod/convec	Convection operator package
actm/gmimod/depos	Deposition operator package
actm/gmimod/depos/include	
actm/gmimod/diffu	Diffusion operator package
actm/gmimod/emiss	Emission operator package
actm/gmimod/emiss/Harvard	Harvard emission routines
actm/gmimod/emiss/include	
actm/gmimod/emiss/llnl	LLNL emission routines

actm/gmimod/in_out	Model input/output routines
actm/gmimod/include	
actm/gmimod/include_data	Include data files
actm/gmimod/mem_manage	Dynamic memory allocation routines
actm/gmimod/phot	Photolysis "operator" package
actm/gmimod/phot/fastj	Fast-J routines
actm/gmimod/phot/include	
actm/gmimod/phot/lookup	Routines implementing the photolysis lookup table
actm/gmimod/phot/utils	
actm/gmimod/step	GMI time stepping routine and control routines for GMI operators
actm/gmimod/trans	UCI transport package
actm/gmimod/trans/include	
actm/gmimod/trans/ucitrans	
actm/gmimod/trans/Uci_Data	
actm/lib	

Table 3: *GMI code directories III*

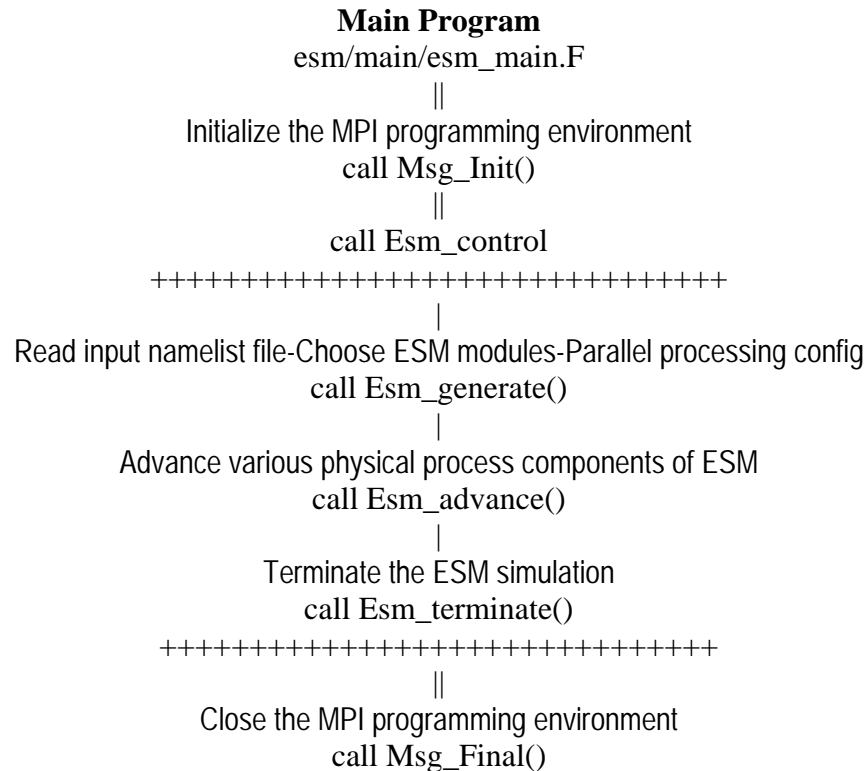| Sub-directories	Description
bin	Location where the executable is placed
doc	General information on gem/ and how it is used
esm	All the esm-level source code and include file. Routines in this directory control and coordinate the functioning of all the other packages
esm/comm	MPI communication routines for ESM
esm/control	Routine defining ESM procedures (generate, advance, terminate)
esm/in_out	Routine reading in the namelisted data for ESM
esm/include	
esm/lib	
esm/main	Main program of the code (esm_main.F)
esm/mem_manage	Routines for dynamic allocations of arrays for ESM
esm/utils	Utility routines such as timing, performance statistics, flushing the buffer, etc.
esm_tools	All the esm_tools source code and include files
esm_tools/baseline	
esm_tools/fi	Routine for assigning unit numbers to input/output files.
esm_tools/include	
esm_tools/lib	
include	General-purpose head files that are used throughout the code. The files contain platform selection, message passing option, compilation options, etc.

Table 4: *GMI code directories IV*

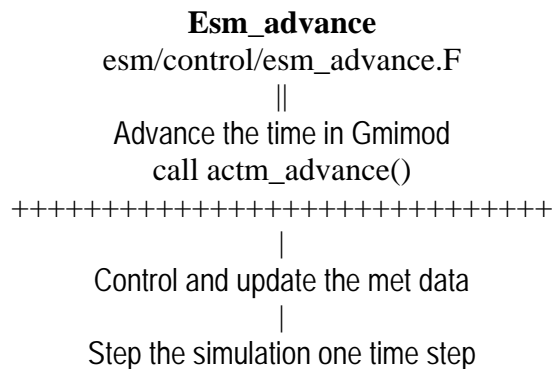## 4- General Flowchart of the Code

In this section, we give through a flowchart the major routines called in the execution of the GMI code. We start from the main program and go down to the GMI time stepping routine.

The main program is Esm_Main (filename ./esm/main/esm_main.F). This calls routines to initialize the MPI programming environment, to control the ESM package and to close the MPI programming environment.

The control routine (Esm_control) for the ESM package calls routines to set up ESM environment (Esm_generate) , to advance physical process components of ESM (Esm_advance) and to terminate the ESM simulation (Esm_terminate).

<div align="center">

Main Program
esm/main/esm_main.F
||
Initialize the MPI programming environment
call Msg_Init()
||
call Esm_control
+++++++++++++++++++++++++++++++++++
|
Read input namelist file-Choose ESM modules-Parallel processing config
call Esm_generate()
|
Advance various physical process components of ESM
call Esm_advance()
|
Terminate the ESM simulation
call Esm_terminate()
+++++++++++++++++++++++++++++++++
||
Close the MPI programming environment
call Msg_Final()

</div>

Esm_advance (called by Esm_control in the main program) is the routine that calls Atmospheric Chemistry Transport Model main driver actm_advance, which in turn calls the main time stepping routine Gmi_Step.
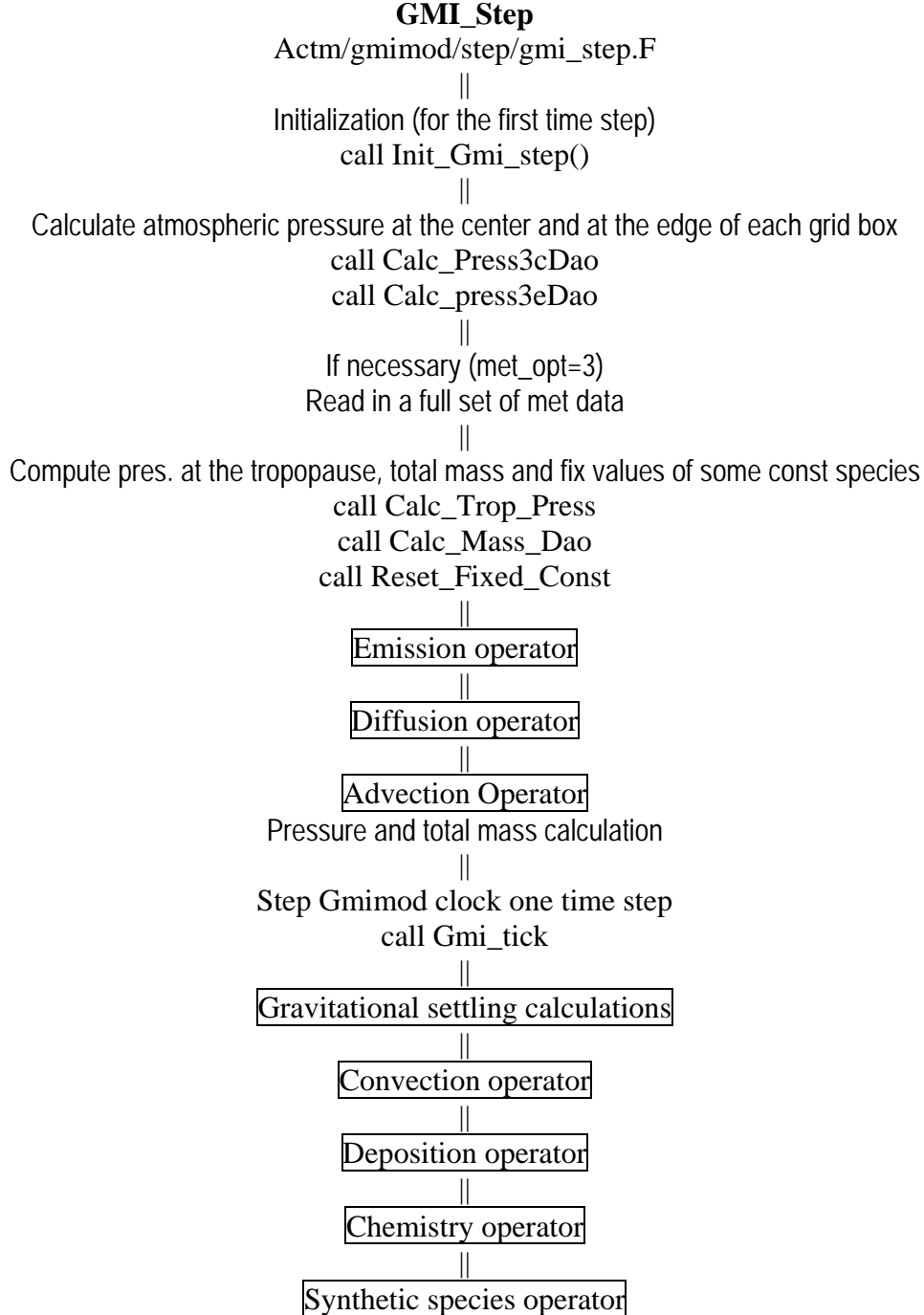
<div align="center">

Esm_advance
esm/control/esm_advance.F
||
Advance the time in Gmimod
call actm_advance()
+++++++++++++++++++++++++++++++
|
Control and update the met data
|
Step the simulation one time step

</div>

5

<div align="center">

call Gmi_step()

+++++++++++++++++++++++++++++++

</div>

Finally, the GMI time stepping control routine GMI_Step (called by actm_advance in Esm_advance) for two transport schemes is given by:

GMI time stepping for LLNLTRANS Transport (trans_opt=1)

<div align="center">

GMI_Step

Actm/gmimod/step/gmi_step.F

||

Initialization (for the first time step)

call Init_Gmi_step()

||

Calculate atmospheric pressure at the center and at the edge of each grid box

call Calc_Press3cDao

call Calc_press3eDao

||

If necessary (met_opt=3)

Read in a full set of met data

||

Compute pres. at the tropopause, total mass and fix values of some const species

call Calc_Trop_Press

call Calc_Mass_Dao

call Reset_Fixed_Const

||

| Emission operator |

||

| Diffusion operator |

||

| Advection Operator |

Pressure and total mass calculation

||

Step Gmimod clock one time step

call Gmi_tick

||

| Gravitational settling calculations |

||

| Convection operator |

||

| Deposition operator |

||

| Chemistry operator |

||

| Synthetic species operator |

</div>

<u>GMI time stepping for UCITRANS Transport (trans_opt=2)</u>

GMI_Step
Actm/gmimod/step/gmi_step.F
||
Initialization (for the first time step)
call Init_Gmi_step()
||
call Uci_control

5- Chemistry Operator Flowchart

For various chemistry options, we present the major routines calls within the chemistry operator.

chem._opt=1, 3, 4, 6

Update_Chem
actm/gmimod/step/chem_update.F
||
Surface area density (SAD) calculations
||
Update the photolysis rate constants qjgmi
call Update_Qj
(The package Fast-J is used here)
||
For chem._opt=1 (randon_lead chemistry)
call Update_Radon_Lead
For chem._opt=3 (simple loss chemistry)
call Update_Loss
For chem._opt=4
call Update_Forc_Bc
For chem._opt=4 (Beryllium chemistry)
call Update_Beryl

chem._opt=7, 8

7

Update_Chem
actm/gmimod/step/chem_update.F
||
| Surface area density (SAD) calculations |
||
Update the photolysis rate constants qjgmi
call Update_Qj
(The package Fast-J is used here)
||
Impose the forcing boundary conditions if they exist
call Update_Forc_BC
||
Calculate the air density at the center of each grid box
||
For chem._opt=7 (Quadchem chemistry)
Call Update_Quadchem
For chem._opt=8 (Sulfur chemistry)
Call Update_Sulfchem

chem._opt=2

Update_Chem
actm/gmimod/step/chem_update.F
||
| Surface area density (SAD) calculations |
||
Update the photolysis rate constants qjgmi
call Update_Qj
(The package Fast-J is used here)
||
Impose the forcing boundary conditions if they exist
call Update_Forc_BC
||
Calculate the air density at the center of each grid box
||
Update the thermal rate constants qkgmi
call Update_Qk
(the setkin routine Kcalc for calculating and returning rate constants is called here)
||
Cycle the chemistry solver using qjgmi and qkgmi
call Update_Smv2chem
||
Accumulate the rates of the photolysis and thermal processes
call Accum_Qqjk
(the setkin routine Calc_Rate_setkin is called here)

Update_Smv2chem
/actm/gmimod/step/chem_update.F
||
Initialization for the ODE solver SmvgearII
call Do_Smv2_Init
||
Change units from mixing ratio to concentration
||
Update const based on surface emissions
call Update_Semiss_Inchem
||
Main control routine for the ODE solver SmvgearII
call Do_Smv2_Solver
||
Change units from concentration back to mixing ratio

Do_Smv2_Solver
Actm/gmimod/chem./smv2chem/smv2chem_solver.F
|||
Solve the gas-phase chemical equations
call physproc
+++
||
Determine block size for chemistry or stiffness
call Deter_Block_Size
||
Solve the chemical ODEs for each block
call Solve_Block
****
|
Set (and rearrange) photofrequencies
|
Compute kinetic reactions and photorates and pressure- and temperature- dependence for gas-
phase chemical reactions
call Calcrate
|
Solve the chemical ODEs
call Smvgear
|

```
Replace block concentrations into domain concentrations
*****************************************
||
Reorder the grid-cells from least to most stiff
call Reorder_Grid_Cells
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

References

1. D.B. Considine, A.R. Douglass, P.S. Connell, D.E. Kinnison, and D.A. Rotman., A polar stratospheric cloud parameterization for the global modeling initiative three dimensional model and its response to stratospheric aircraft, *J. Geo. Res*., **105**(D3), p. 3955-3973 (2000).
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